Isopropyl ether

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 29.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.04e-01

Confidence level: 7.18e-01

Nearest Neighbors from the Training Set

Image not found
1-Pentanol
Measured: 5.01
Predicted: 7.31

Image not found
3-Methylaniline
Measured: 33.9
Predicted: 33.3

Image not found
N-Methylaniline
Measured: 191
Predicted: 109

Image not found
1-Hexanol
Measured: 10.2
Predicted: 11.9

Image not found
4-Methylaniline
Measured: 79.4
Predicted: 104